REPORT DOCUMENTATION PAGE

Form Approved
OMB No. 0704-0188

1. REPORT DATE *(DD-MM-YYYY)*
09-04-2009

2. REPORT TYPE
Final Performance Report

3. DATES COVERED *(From - To)*
Jan 2005-Dec 2007

4. TITLE AND SUBTITLE
Design of Phononic Micro/Nanostructures for Harsh Environments

5a. CONTRACT NUMBER
FA9550-05-1-0046

5b. GRANT NUMBER

5c. PROGRAM ELEMENT NUMBER

6. AUTHOR(S)
Martin L. Dunn

5d. PROJECT NUMBER

5e. TASK NUMBER

5f. WORK UNIT NUMBER

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)
University of Colorado
Boulder, CO

8. PERFORMING ORGANIZATION REPORT NUMBER

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)
Air Force Office of Scientific Research
875 North Randolph Street
Arlington, VA22203

10. SPONSOR/MONITOR'S ACRONYM(S)

11. SPONSOR/MONITOR'S REPORT NUMBER(S)
AFRL-OSR-VA-TR-2013-0909

12. DISTRIBUTION/AVAILABILITY STATEMENT
Distribution Statement A: Approved for public release. Distribution is unlimited.

13. SUPPLEMENTARY NOTES

14. ABSTRACT

With this support we developed, implemented, and validated a suite of computational tools for the optimal design of phononic materials using topology optimization.
Specifically we have:

- Developed an analysis and optimization code to handle large sized 3D elastic wave propagation problems in heterogeneous media by implementing a
parallel solver to handle large systems described by complex-valued systems of equations.
- Verified our ideas and tested the code on a number of numerical examples in 2D and 3D.
- Studied many problems regarding 2D and 3D bulk and surface waves and their use to create wave guiding devices.
- Developed and implemented an approach to design phononic bandgap materials on a periodic cell.

15. SUBJECT TERMS

16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT	18. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON
a. REPORT	b. ABSTRACT	c. THIS PAGE			19b. TELEPHONE NUMBER *(Include area code)*
					303-496-6542

Final Report

Project Name: Design of Phononic Micro/Nanostructures for Harsh Environments

Agreement No: AFOSR FA9550-05-1-0046

Time Frame: Jan 05-Dec 07

Project participants	Project/Organization Role
Martin L. Dunn	Professor, Dept. of Mechanical Engineering, PI
Kurt Maute	Professor, Dept. of Aerospace Engineering Sciences, PI
Anton Evgrafov	Research Associate, Dept. of Aerospace Engineering Sciences
Cory Rupp	Ph.D. student, Dept. of Mechanical Engineering

1 Summary

With this support we developed, implemented, and validated a suite of computational tools for the optimal design of phononic materials using topology optimization. Specifically we have:

- Developed an analysis and optimization code to handle large sized 3D elastic wave propagation problems in heterogeneous media by implementing a parallel solver to handle large systems described by complex-valued systems of equations.
- Verified our ideas and tested the code on a number of numerical examples in 2D and 3D.
- Studied many problems regarding 2D and 3D bulk and surface waves and their use to create wave guiding devices.
- Developed and implemented an approach to design phononic bandgap materials on a periodic cell.
- Used our computational tools to study the potential of elastic wave guides as logic devices.

The results have been/will be presented at:

- 2005 ASME International Mechanical Engineering Congress and Exposition (held on November 2005, in Orlando, FL).
- 2006 International Conference on Composites/Nano Engineering (Jul. 2006, Broomfield, CO).
- 2006 AIAA/ISSMO Multidisciplinary Analysis and Optimization Conference (Sept. 2006, Portsmouth, VA).
- 2006 Graduate Engineering Annual Research Symposium (Mar. 2006, Boulder, CO).

- 2006 ASME International Mechanical Engineering Congress and Exposition (November, 2006, in Chicago, IL).
- 7th World Congress on Structural and Multidisciplinary Optimization, May 21-25, 2007, Seoul, Korea.

2 Objectives

While the quasi-static behavior of materials and devices is of vital importance, the dynamic behavior can be even more significant for microsystems applications. For example, design goals for RF systems are focused on tailoring the resonance spectrum. Inexpensive, batch-fabricated chemical and biological sensors can be enabled by micromachined wavelength-selective emitter/bolometer arrays, but these must be precisely thermally isolated (heat is conducted by phonons). Micromachined acoustic sensors, for example, for damage detection in a high-temperature turbine, require high-resolution incoming waves. Vibration isolation and shock protection of microsystems pose significant and largely unsolved problems. Tailoring of dispersion properties of materials, in particular the design of phononic band gap materials, and the design of structures with specific wave guiding and absorption features has recently attracted substantial interest. Concerning the design of materials, the bulk of the work has focused so far on theoretical and experimental studies on the physics of band gaps in periodic materials (Sigalas and Economou, 1992; Vasseur et al. 1998; Liu et al., 2000). It was shown that the transparency of a material for elastic waves can be altered by augmenting a soft matrix material by stiffer inclusions. Only little work, however, has been done on systematic design approaches to design band gap materials. Cox and Dobsen (1999, 2000) first exploited the potential of topology optimization for the design of photonic band-gap materials. For elastic waves, Sigmund and Jensen (2003) and Hussein et al., (2003; 2004) have studied the optimum topology of unit cells in infinite periodic media. The same research groups have also studied waveguides and filters for bulk in-plane elastic and acoustic waves, using periodic microstructures. Hussein et al., (2003; 2004) created defects in periodic materials to guide waves, while Sigmund and Jensen (2003) developed a topology optimization approach to accomplish this.

Our objective is to develop an approach to design the layout of multiple constituent materials that are distributed in distinct, often non-intuitive, complex patterns to create materials and devices with tailored phononic properties. We generate these patterns using topology optimization, building on our previous and ongoing efforts to develop a general purpose analysis and design tools.

3 Status of Effort

We made excellent progress during this effort. Our main efforts are along two lines: i) computational method development and implementation, and ii) applications. During this research we:

- Developed, implemented, and validated a topology optimization approach for 2D and 3D wave propagation problems, including a version with a parallel solver.
- Developed, implemented, and validated a topology optimization approach for 2D phononic bandgap materials.
- Applied the methodology to numerous design problems involving 2D and 3D bulk and surface waves, and 2D phononic bandgap materials.

- Applied the methodology to the design of phononic wave devices to function as logic devices.
- Developed an analysis and design approach to study the effect of active deformation on wave propagation characteristics in phononic bandgap materials and wave guiding devices.

4 Accomplishments/New Findings

Topology Optimization Approach

In topology optimization of phononic materials, the computational domain is discretized into a grid of finite elements on which the elastic wave equation is solved. The general optimization problem which is specialized for the harmonic wave equation is as follows:

$$\begin{aligned} &\min_{s_i} \; z(s_i, \mathbf{u}(s_i)) && 0 < s_i \le 1 \\ &s.t. \; \left([\mathbf{K}] + i\omega[\mathbf{C}] - \omega^2[\mathbf{M}]\right)\mathbf{u} - \mathbf{f} = 0 && \\ &\quad g_j(s_i, \mathbf{u}(s_i)) \le 0 && j = 1,2,3\ldots \\ &\quad h_k(s_i, \mathbf{u}(s_i)) = 0 && k = 1,2,3\ldots \end{aligned} \tag{1}$$

In eqs. (1), z is the objective function, $\mathbf{u}$ is vector of displacements that is the solution of the finite element problem, s_i are design variables which define the material properties for each element, [**K**], [**C**], and [**M**] are the stiffness, damping, and mass matrices, respectively, ω is the driving frequency for the forcing vector **f**, and g_j and h_k are constraints on the problem. The objective function can take many different forms, but for the phononic problems, the following formulation with its analytically derived sensitivities seems to work well:

$$\begin{aligned} &z = (\bar{u})^T L\, u \\ &\frac{dz}{ds_i} = 2 \cdot \mathrm{Re}\left([L]\bar{u}\right)^T \left(-[\tilde{K}]^{-1}\right) \frac{\partial[\tilde{K}]}{\partial s_i} u \end{aligned} \tag{2}$$

where:

$$\begin{aligned} &[\tilde{K}] = [K] + i\omega[C] - \omega^2[M] \\ &\frac{\partial[\tilde{K}]}{\partial s_i} = \frac{\partial[K]_e}{\partial s_i} + \omega\frac{\partial[C]_e}{\partial s_i} - \omega^2\frac{\partial[M]_e}{\partial s_i} \end{aligned} \tag{3}$$

This objective function maximizes the norm of the displacements at degrees of freedom determined by L. This formulation results an optimization problem for which the sensitivities are easy to compute.

In order to determine the layout of different materials in the domain, the material properties for the i-the element (elastic constants, density) are varied continuously as a function of the design variables s_i. We use a simple linear variation between the two materials of interest, but it is straightforward to use a penalty formulation or other similar techniques. In each iteration of the optimization algorithm a new value for each s_i is determined based on its value and the corresponding sensitivity. At the end of each iteration the objective function will be improved and eventually the design variables will reach or approach the box constraints. When all or most of the variables reach the box constraints the optimum phononic material is achieved. We solve the optimization problems using sequential convex programming (SCP) with the method of moving asymptotes (MMA). No constraints, other than the box constraints, exist on the problems.

Parallel Implementation - Domain Decomposition Approach

In order to efficiently perform repeated 3D finite element analyses of surface wave problems arising at every optimization iteration we employ a parallel solver. The basic idea behind solving linear systems arising from finite element discretizations of partial differential equations on modern distributed memory parallel computers is "divide and conquer." The elastic solid, occupying the computational domain, is divided into non-overlapping regions (see Figure 1):

$$\Omega = \bigcup_k \Omega_k$$

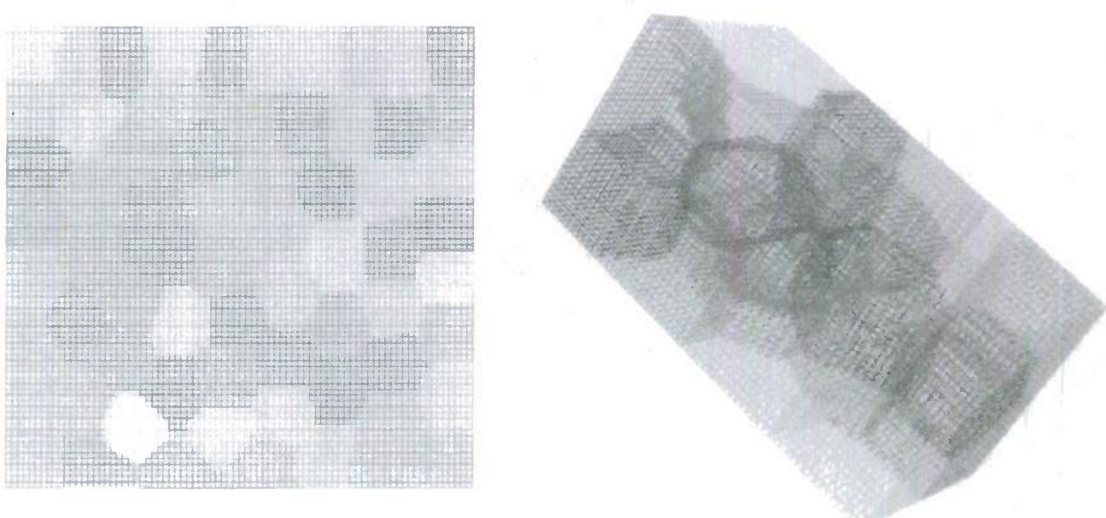

Fig. 1 Domain decomposition in two and three dimensions.

Such a decomposition naturally induces a subdivision of the finite element mesh. Thus, all finite element quantities, such as the solution and the load vectors, as well as the stiffness, mass, and damping matrices may be restricted to each subregion, or subdomain:

$$K_{ij} = \int_\Omega (\nabla\varphi_i, A(x)\nabla\varphi_j)dx = \int_{\Omega_k} (\nabla\varphi_i, A(x)\nabla\varphi_j)dx \text{ , where } \Omega_k \supseteq \operatorname{supp}(\varphi_i)\bigcup \operatorname{supp}(\varphi_j)$$

Therefore, using the domain decomposition technique we transform the wave propagation problem in the whole solid into wave propagation sub-problems in each subdomain, coupled only through the constraints imposing continuity of the global solution across the subdomain interface.

$$[B]u = 0$$

These constraints are imposed weakly, through the Lagrange multiplier technique, so we have to solve the following linear system:

$$([K]+i\omega[C]-\omega^2[M])u+[B]^T\lambda=f$$
$$[B]u=0$$

Now the primal variables u may be completely excluded from the system above by solving the wave propagation problem locally on each subdomain in parallel, and then the resulting system of dual equations in λ is solved using an efficiently preconditioned parallel iterative solver.

At the level of the optimization algorithm, we chose not to parallelize the code owing to the special structure of the topology optimization problems, where the number of state variables (displacements) grows much faster (as n^3 for a cubical domain of size n) than the number of design variables (which is n^2 for a cubical domain of size n). Thus we take a "master node" approach, where only one selected node in a computational cluster is concerned with optimization, and contains all design variables. Thus, the algorithm works as follows:

1. Choose an initial design x_0, set k=0.
2. Send the material properties based on x_k from the master node to the rest of the computational nodes; compute the displacements $u(x_k)$ a domain decomposition algorithm outlined above. Evaluate the objective function $f(x_k, u(x_k))$ and its gradient $\partial f(x_k, u(x_k))$ using parallel computing and collect the values on the master node.
3. On the master node, compute $x_{k+1} = x_k - \alpha_k \partial f(x_k, u(x_k))$,
4. Check whether convergence is attained; if not, set k = k +1 and go to step 2.

Nonlinear Strain Effects for a Switchable Waveguide

As a mean of tuning/controlling the wave-guide, finite prestraining may be implemented in various ways, including but not limited to thermal or mechanical loading, or electric loading when used in conjunction with piezo-electric materials. To demonstrate, we used mechanically induced finite pre-straining to illustrate the concept of designing tunable elastic wave-guides with predefined functional properties. We assume that two scales are present in the non-linear dynamics model describing the behaviour of the wave-guide in the deformed configuration. Time-independent loads necessary to achieve the finite deformation of the wave-guide are much larger than the harmonic loads used as an "input signal" to the wave-guide. So we assume the following decomposition of the traction:

$$\mathbf{t}(\mathbf{x},t)=\mathbf{t}^{nl}(\mathbf{x},t)+\varepsilon\mathbf{t}^{harm}(\mathbf{x},t)$$

where e > 0 is a small scale parameter. We also assume that the displacement fields involved in the problem may be decomposed in a similar manner:

$$\mathbf{u}(\mathbf{x},t)=\mathbf{u}^{nl}(\mathbf{x},t)+\varepsilon\mathbf{u}^{harm}(\mathbf{x},t)$$

We drop from the equations of elasticity all the terms involving strain squared, which in turn allows us to bypass solving the underlying non-linear dynamics problem to find u(x, t), and instead we solve a non-linear static problem to determine $\mathbf{u}^{nl}(\mathbf{x},t)$ and then separately solve a linear quasi-static problem to find the Fourier transformation of $\mathbf{u}^{harm}(\mathbf{x},t)$ in the deformed configuration. Complete details can be found in Evgrafov et al, (2008).

Applications

We have applied the topology optimization approach to a number of fascinating problems including:

- 2D Bragg grating
- 2D Waveguide (bender)
- 2D Pressure wave to shear wave mode converter (phononic inverter)
- 2D Phononic switch
- 2D Phononic multiplexer (sort frequencies or wave types)
- 2D Surface wave filter with bandgap maximization
- 3D Bragg grating
- 3D Surface source waveguide
- 3D Bending waveguide
- 2D Bandgap meta-materials design:
    - bulk meta-materials for device
    - plate/beam meta-materials for structural applications

These problems can be grouped into three different types, namely 1) those that are a direct attempt toward the development of elastic logic, 2) those affecting the propagation of surface waves, and 3) those for the design of bandgap meta-materials.

In the pursuit of the design of elastic logic devices it has been necessary to investigate different methods to serve this purpose. Two options include the on/off method and a new idea the mode conversion method. The on/off method follows a similar route as that for electronic circuits in that the state depends on whether the signal is present or not. This resulted in the design of a 2D phononic switch in which depending on the state of two input ports the elastic wave would exit one of two output ports. The second method is based on an idea that the mode of the wave (pressure or shear wave) acts as the on or off state. This idea resulted in the design of a 2D phononic inverter which converts one wave type into another and the design of a phononic multiplexer which sorts incoming waves by type into different output ports. Both methods have shown promise in reaching the larger goal of the design of elastic logic.

Surface wave device design has been a major focus because of their applicability to real device designs. A current practical example is Surface Acoustic Wave filters used in may electronics applications. We reproduce a similar device and improve on its basic design by optimizing the bandgap at which it operates. Our interest extends further than that, however, to the design of 3D surface waveguides which direct the propagation of surface waves in a similar manner as the 2D examples and may as well lead to elastic surface wave logic devices. A particularly challenging example has been the 3D waveguide shown in Fig. 2. A half-space is approximated computationally with the use of wave energy absorbing boundary conditions into which a surface wave propagates in a predetermined direction. In a homogenous material the surface wave passes through the computational domain unimpeded. In this problem, however, it is desirable to have the wave exit the domain at a location perpendicular to the entrance location thereby requiring the wave to bend a corner. The optimization problem is set up such that the displacements are maximized at an output location. This problem has been solved before as a topology optimization problem by Bendsoe and Sigmund (2003) for bulk waves using a two-dimensional model but has never been done for surface waves in three dimensions. The results of this problem can be seen in the figure which shows isosurfaces located at the interface between the two design materials silicon (blue) and aluminum (red). The topology of the design is non-intuitive but can be imagined it guides the surface wave by reflecting it off of the curved surfaces in some complex manner.

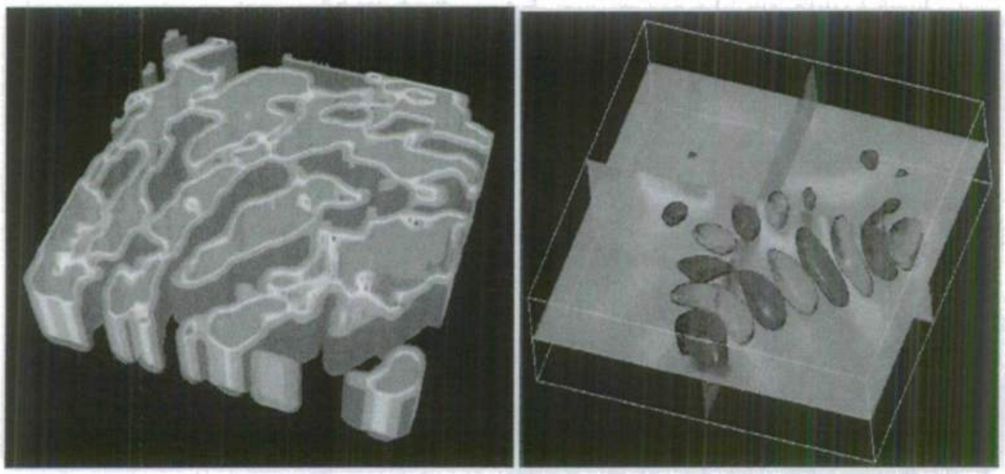

Fig. 2 Final design of a 3D surface wave bending waveguide (left) causes an incoming surface wave to bend a corner (right).

We also worked extensively to design bandgap meta-materials through which elastic waves of certain frequencies will not propagate. These meta-materials are based on arrayed unit cell structures. It is the design of structure of the unit cell that determines which waves will propagate and which will not. So far we have designed frequency filtering 2D bulk meta-materials as well as plate/beam structures which serve the same purpose; an example is shown in Fig. 3.

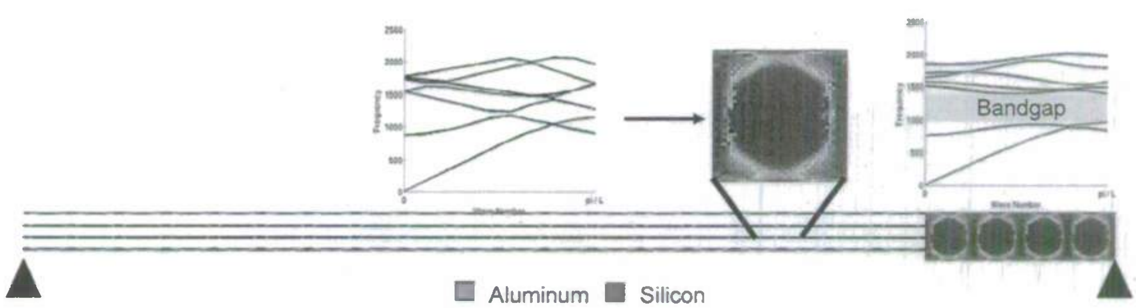

Fig. 3 Design of a bandgap meta-material designed to have a bandgap at a prescribed frequency range.

Such technology is currently promising because of its application to materials with a negative refraction index which have been shown to allow for the design of such things as invisibility cloaks or superlenses. The advantage we have is that unlike over current groups in this research area we have the ability to design for an optimal unit cell.

5 Personnel Supported

This grant has supported the PI and co-PI (Dunn and Maute) for one month of summer salary, and we have also partially supported Dr. Anton Evgrafov as a research associate. Cory Rupp, a graduate student at CU, has also worked on this project and was supported by an NSF fellowship for part of the project

6 Publications

Evgrafov, A., Rupp, C. J., Dunn, M. L., and Maute, K., 2008, "Optimal Synthesis of Tunable Elastic Waveguides," *Computer Methods in Applied Mechanics and Engineering*, Vol. 198, pp. 292-301.

Evgrafov, A., Rupp, C. J., Maute, K., and Dunn, M. L., 2008, "Large-Scale Parallel Topology Optimization Using a Dual-Primal Substructuring Solver," *Structural and Multidisciplinary Optimization*, Vol. 36, pp. 329-345.

Rupp, C. J., Evgrafov, A., Maute, K., and Dunn, M. L., 2007, "Design of Phononic Materials/Structures for Surface Wave Devices Using Topology Optimization," *Structural and Multidisciplinary Optimization*, Vol. 34, pp. 111-121.

Rupp, C., Frenzel, M., Evgrafov, A., Maute, K., and Dunn, M. L., 2005, Design of Nanostructured Phononic Materials," in *Proceedings of the ASME IMECE 2005*, IMECE2005-82206.

Rupp, C. J., Evgrafov, A., Dunn, M. L., and K. Maute, "Large-Scale Topology Optimization of Phononic Meta-Materials for Surface Wave Devices," in Proceedings of 7th World Congress on Structural and Multidisciplinary Optimization, May 21-25, 2007, Seoul, Korea. (Selected as Finalist for Best Paper Award)

Rupp, C. J., Evgrafov, A., Maute, K., Dunn, M. L., 2006, "Design of Phononic Nanostructured Materials and Structures Using Topology Optimization," in Proc. 2006 International Conference on Composites/Nano Engineering.

Rupp, C. J., Evgrafov, A., Maute, K., Dunn, M. L., 2006, "Design of Phononic Surface Wave Devices Using Topology Optimization," in Proc. Of the AIAA/ISSMO Multidisciplinary Analysis and Optimization Conference 2006.

Rupp, C. J., Evgrafov, A., Maute, K., Dunn, M. L., 2006, "Design of Phononic Materials/Structures Using Topology Optimization," in Proc. of the ASME IMECE 2006, IMECE2006-15071.

Dunn, M. L., Maute, K., Evgrafov, A., and Rupp, C., 2005, "Design of Phononic Micro/Nanostructures for Harsh Environments," in Proc. 2005 AFOSR Mechanics of Materials and Devices Contractors Meeting.

7 Interactions/Transitions

Results of this research have been/will be presented at:

- 2005 AFOSR Contractors Meeting (Santa Fe, NM, Aug. 2005), oral presentation.
- 2005 ASME International Mechanical Engineering Congress and Exposition (Orlando, FL, Nov. 2005).
- 2006 ASME International Mechanical Engineering Congress and Exposition (Chicago, IL, Nov. 2006).
- Project results were presented to and discussed with the Program Manager, Dr. Clark Allred at a visit to CU in April 2006.
- 2006 AFOSR Contractors Meeting (Seattle, WA, Aug. 2006), to be presented as a poster.
- 11th AIAA/ISSMO Multidisciplinary Analysis and Optimization Conference (Sep 6-8, 2006).
- 2006 International Conference on Composites/Nano Engineering (Jul. 2006, Broomfield, CO).
- 7th World Congress on Structural and Multidisciplinary Optimization, May 21-25, 2007, Seoul, Korea.
- ASME IMECE 2006, IMECE2006-15071.

8 Discoveries, Inventions, or Patent Disclosures

None

9 Honors/Awards

- Cory Rupp won best presentation awards at the annual Graduate Engineering and Research Symposium at CU in 2006 and 2007.
- Martin L. Dunn was awarded the Victor Schelke Endowed Chair at CU.
- Kurt Maute was awarded the College of Engineering Joseph H. Smead Faculty Fellowship at CU.
- Martin L. Dunn was elected a Fellow of the American Society of Mechanical Engineers
- Our paper "Large-Scale Topology Optimization of Phononic Meta-Materials for Surface Wave Devices," in Proceedings of 7th World Congress on Structural and Multidisciplinary Optimization, May 21-25, 2007, Seoul, Korea was selected as Finalist for Best Paper Award.